

APPLICATION OF FOURTH ORDER VIBRATIONAL PERTURBATION THEORY WITH ANALYTIC HARTREE-FOCK FORCE FIELDS

JUSTIN Z GONG, DEVIN A. MATTHEWS, *Department of Chemistry and Biochemistry, The University of Texas, Austin, TX, USA*; JOHN F. STANTON, *Department of Chemistry, The University of Texas, Austin, TX, USA*.

Fourth-Order Rayleigh-Schrodinger Perturbation Theory (VPT4) is applied to a series of small molecules. The quality of results have been shown to be heavily dependent on the quality of the quintic and sextic force constants used and that numerical sextic force constants converge poorly and are unreliable for VPT4. Using analytic Hartree-Fock force constants, it is shown that these analytic higher-order force constants are comparable to corresponding force constants from numerical calculations at a higher level of theory. Calculations show that analytic Hartree-Fock sextic force constants are reliable and can provide good results with Fourth-Order Rayleigh-Schrodinger Perturbation Theory.